Lattice simulations of the QCD chiral transition at real baryon density

Towards lattice QCD at not so small baryon densities

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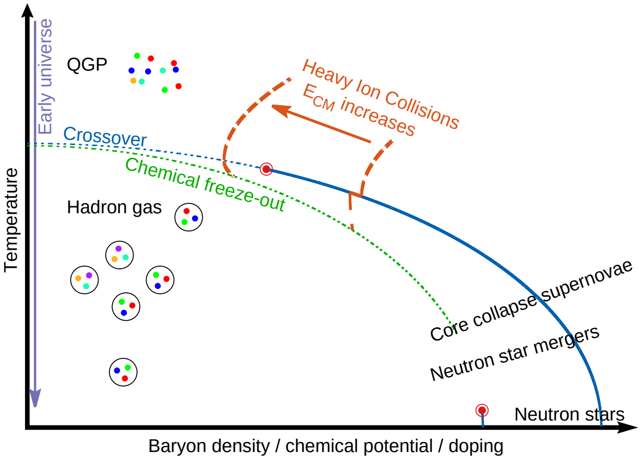
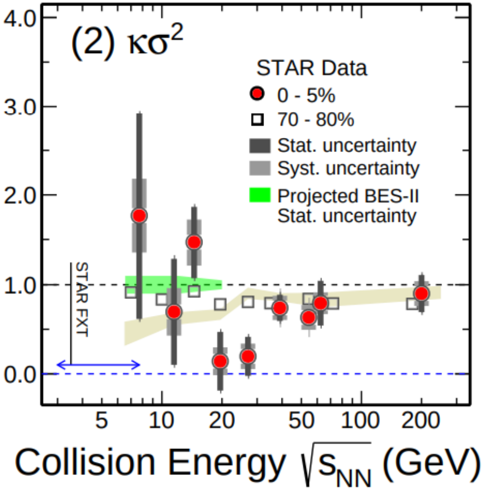
2004.10800 [hep-lat]; JHEP 05 (2020) 088; Giordano, Kapas, Katz, Nogradi, Pasztor
2108.09213 [hep-lat]; Borsanyi, Fodor, Giordano, Katz, Nogradi, Pasztor, Wong

The conjectured phase diagram of QCD



The experimental search for the CEP



STAR, PRL126 (2021) 9, 092301; from abstract: "models of heavy-ion collisions without a critical point show a monotonic variation as a function of s_{NN}"

Minimum at: $\sqrt{s_{NN}} = 19.6\text{GeV} \to \mu_B \approx 200\text{MeV}$ and $\mu_B/T \approx 1.3$
Lowest energy: $\sqrt{s_{NN}} = 7.7\text{GeV} \to \mu_B \approx 400\text{MeV}$ and $\mu_B/T \approx 3$
It would be nice to say something from first principle calculations.

Why is finite μ_B so difficult for the lattice?

Lattice QCD is a set of theoretical and computational techniques to perform the Euclidean path integral:

$$Z = \int \mathcal{D}A_\mu \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\frac{1}{4}\int F_{\mu\nu}F_{\mu\nu} - \int \bar{\psi}(\gamma_\mu \partial_\mu + \gamma_0 \mu + m)\psi}$$

we integrate out the fermions analytically, to get

$$Z = \int \mathcal{D}A_\mu \det M(A_\mu, \mu, m)\psi e^{-\frac{1}{4}\int F_{\mu\nu}F_{\mu\nu}}$$

where M is (a discretized version of) the Dirac-operator. We can simulate this with Monte Carlo techniques if $\det M$ is **real and positive**:

- chemical potential $\mu = 0$
- purely imaginary chemical potentials: $\mathrm{Re}\,\mu = 0$
- isospin chemical potential: $\mu_u = -\mu_d$

Otherwise: **complex action or sign problem**
$\rightarrow$ desperate times, desperate measures

Approaches to finite density lattice QCD

Known approaches that try to side-step the complex action problem introduce additional serious problems. E.g.

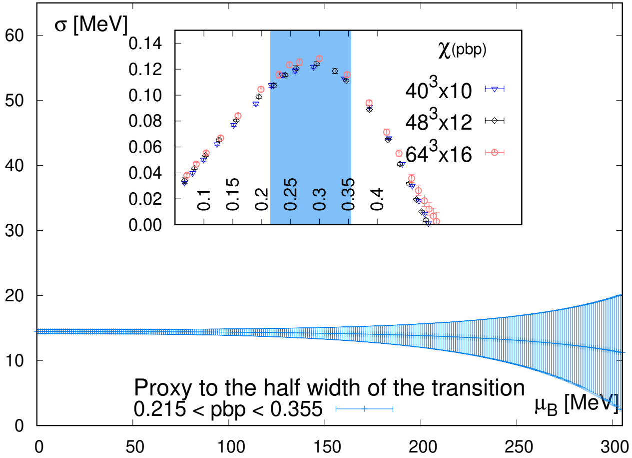
- Taylor and imaginary μ: **analytic continuation problem**
- Reweighting and Taylor: **overlap problem**
- Complex Langevin: **convergence issues**
- ...

This talk:

$\rightarrow$ a direct method

There is a sign problem, but if it is dealt with by sufficient statistics, the results are reliable, and errors (on a fixed lattice setup) are statistical only.

Trying to look for criticality with analytic continuation



PRL 125 (2020) 5, 052001; Borsanyi, Fodor, Guenther, Kara, Katz, Parotto, Pasztor, Ratti, Szabo

Unpredictive in the phenomenologically interesting range from $\mu_B/T = 1.3 \ldots 3$

Reweighting: in general

Target theory: Z_w Simulated theory: Z_r

$$Z_w = \int \mathcal{D}U\ w(U) \qquad w(U) = detM[U,\mu]e^{-S_g[U]} \in \mathbb{C}$$

$$Z_r = \int \mathcal{D}U\ r(U) \qquad r(U) > 0$$

$$\frac{Z_w}{Z_r} = \left\langle \frac{w}{r} \right\rangle_r$$

$$\langle O \rangle_w = \frac{\int \mathcal{D}U\ w(U)O(U)}{\int \mathcal{D}U\ w(U)} = \frac{\int \mathcal{D}U\ r(U)\frac{w(U)}{r(U)}O(U)}{\int \mathcal{D}U\ r(U)\frac{w(U)}{r(U)}} = \frac{\left\langle \frac{w}{r} O \right\rangle_r}{\left\langle \frac{w}{r} \right\rangle_r}$$

Two problems that are exponentially hard in the volume:

- $\frac{w}{r} \in \mathbb{C} \rightarrow$ the complex action problem became a **sign problem**
- Tails of $\rho(\frac{w}{r})$ long $\rightarrow$ **overlap problem**

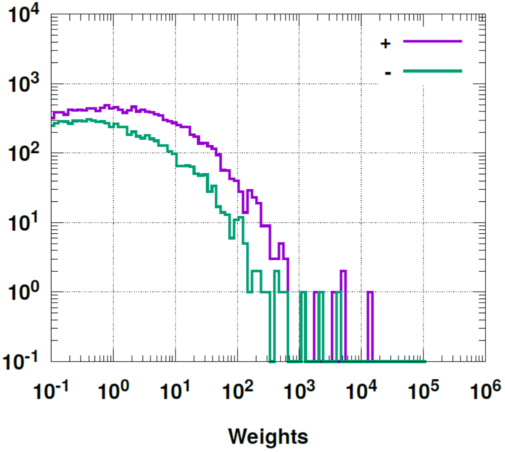
An old lattice estimate of the crit. pt. comes from reweighting from $\mu = 0$ on very coarse lattices: Fodor, Katz; JHEP 04 (2004) 050

Why does reweighting from $\mu = 0$ fail?

The expectation value of any observable:

$$\langle O \rangle_w = \frac{\left\langle \frac{w}{r} O \right\rangle_r}{\left\langle \frac{w}{r} \right\rangle_r}$$

The weights are the $\frac{w}{r} \propto \frac{\det M(\mu)}{\det M(0)}$. To calculate anything, we need to have control over the observable



The **sign problem is under control, the overlap problem is not:**
Giordano, Kapas, Katz, Nogradi, Pasztor; PRD 102, 034503 (2020)

Phase reweighting

A simple way to avoid long tails for the distribution of $\frac{w}{r}$ is to make sure that w/r come from a compact space. E.g.

$$\begin{aligned} w &= e^{-S_g} \det M = e^{-S_g} |\det M| e^{i\theta} \\ r &= e^{-S_g} |\det M| \end{aligned} \quad \Rightarrow \quad \frac{w}{r} = e^{i\theta}$$

Some studies, e.g. Fodor, Schmidt, Katz; JHEP 03 (2007) 121
Endrodi, Fodor, Katz, Sexty, Szabo, Torok; PRD 98 (2018) 7,074508
Not pursued in large scale studies.

Common lore:

- PQ: $|\det M| = |\det M_u(\mu) \det M_d(\mu)| = \det M_u(\mu) \det M_d(-\mu)$
  $\rightarrow$ isospin chemical potential
- pion condensation for $\mu_q \gtrapprox \frac{m_\pi}{2}$
- $\left\langle e^{i\theta} \right\rangle_{PQ} = \frac{Z_{\mu_B}}{Z_{\mu_I}} = e^{-V(F_B - F_I)} \rightarrow$ severe sign problem

Sign reweighting

$$Z = \int \mathcal{D}U e^{-S_g} \det M = \int \mathcal{D}U e^{-S_g} \mathrm{Re} \det \mathrm{M}$$

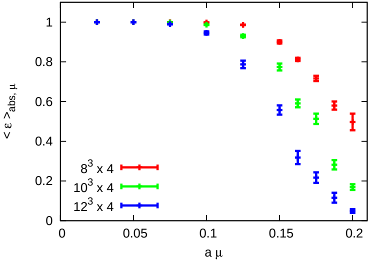
- Beware: the substitution $\det M \to \mathrm{Re} \det M$ can be done in Z but not in generic expectation values.
- E.g. things like $\frac{\partial^n \log Z}{\partial \mu_{ud}^n}$, $\frac{\partial^n \log Z}{\partial m_{ud}^n}$ and $\frac{\partial^n \log Z}{\partial \beta^n}$ can be calculated

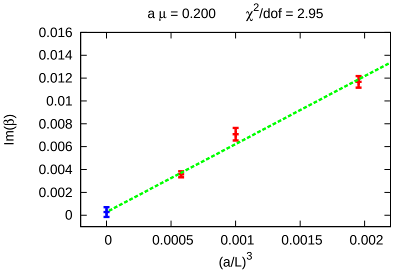
A new choice of a theory to reweight to and from:

$$\begin{aligned} w &= e^{-S_g} \mathrm{Re} \det \mathrm{M} \\ r &= e^{-S_g} \left| \mathrm{Re} \det \mathrm{M} \right| \end{aligned} \quad \Rightarrow \quad \frac{w}{r} = \mathrm{sgn} \cos \theta = \pm 1$$

- The weights are $\epsilon = \pm 1 \to$ No tail, **no overlap problem**
- $\langle \pm \rangle_r$ measures the strength of the **sign problem**
- de Forcrand, Kim, Takaishi; Nucl. Phys. B Proc. Suppl. 119, 541 (2003) $\to$ optimal choice for $\frac{w}{r} = f(\theta)$
- But: hard to simulate with weights $\propto |\mathrm{Re} \det \mathrm{M}|$

Numerical test - unimproved staggered at $N_\tau = 4$





JHEP 05 (2020) 088; Giordano, Kapas, Katz, Nogradi, Pasztor
Consistent with the 2004 paper. BUT: to start being relevant for phenomenology, a much better lattice action has to be used

Understanding the strength of the sign problem

The strength of the sign problem is governed by the same underlying probability distribution:

$$P_{PQ}(\theta) = \langle \delta(\theta - \mathrm{Arg}(\det M)) \rangle_{PQ}$$

With a known P_{PQ} we have:

$$< \cos\theta >_{PQ} = \int_{-\pi}^{+\pi} P_{PQ}(\theta) \cos\theta d\theta$$

$$< \mathrm{sgn} \cos\theta >_{SQ} = \frac{\int_{-\pi}^{+\pi} P_{PQ}(\theta) \cos\theta d\theta}{\int_{-\pi}^{+\pi} P_{PQ}(\theta) |\cos\theta| d\theta}$$

2-step approximation:
(i) leading order cumulant: $P_{\mathrm{PQ}}(\theta) \sim$ wrapped Gaussian
(ii) leading order Taylor $\left\langle \theta^2 \right\rangle_{\mathrm{LO}} = -\frac{4}{9} \chi_{11}^{ud} \left(LT\right)^3 \hat{\mu}_B^2$
QCD input: $\chi_{11}^{ud} = \frac{1}{T^2} \frac{\partial^2 p}{\partial\mu_u \partial\mu_d}|_{\mu=0}$

Analytic formulas for the asymptotic behavior

Weak sign problem: small μ or V

$$\langle \cos\theta \rangle^{\mathrm{PQ}}_{T,\mu} \sim 1 - \frac{\sigma^2(\mu)}{2}$$

$$\langle \varepsilon \rangle^{\mathrm{SQ}}_{T,\mu} \sim 1 - \left(\tfrac{4}{\pi}\right)^{\frac{5}{2}} \left(\frac{\sigma^2(\mu)}{2}\right)^{\frac{3}{2}} e^{-\frac{\pi^2}{8\sigma^2(\mu)}}$$

$< \operatorname{sgn}\cos\theta >_{SQ}$ approaches 1 faster than any polynomial.

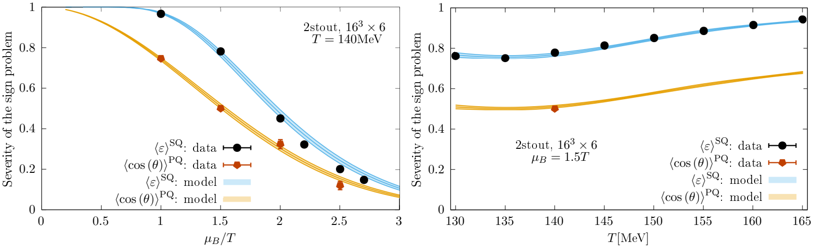
Strong sign problem: large μ or V

$$\frac{\langle \varepsilon \rangle^{\mathrm{SQ}}_{T,\mu}}{\langle \cos\theta \rangle^{\mathrm{PQ}}_{T,\mu}} \sim \frac{\pi}{2}\,,$$

$\rightarrow$ a factor of $(\frac{\pi}{2})^2 \approx 2.5$ in statistics asymptotically

There is a chance for a window at intermediate chemical potentials, where the sign problem with sign quenched is still weak.

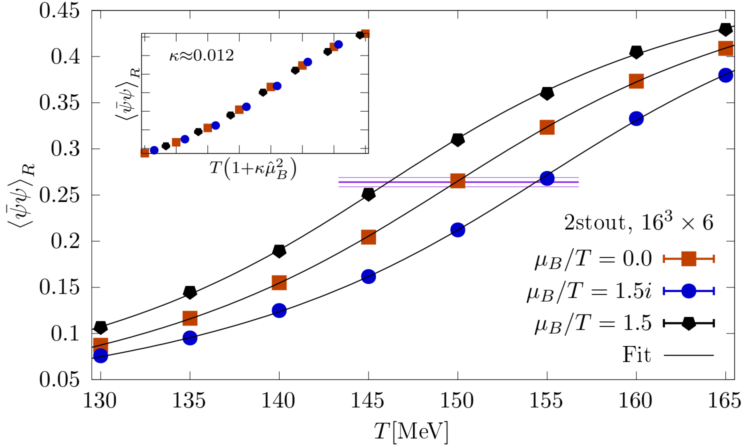
The simulated strength of the sign problem



- Statistics required $\propto 1/(\text{strength of the sign problem})^2$
- Small μ model describes actual data pretty well
- Const. strength of the sign problem for const. $(LT)^3\left(\frac{\mu_B}{T}\right)^2$ (roughly)
- For $LT = 16/6 \approx 2.7$ the sign problem is managable for the entire RHIC Beam Energy Scan range

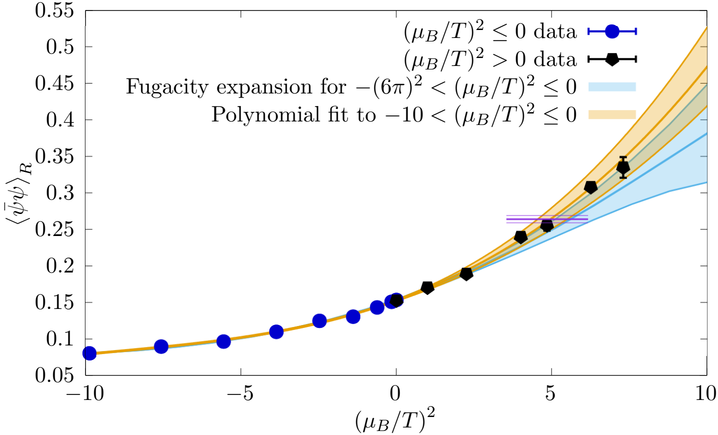
Temperature scan - 2stout improved $N_\tau = 6$

$$\langle\bar{\psi}\psi\rangle_R = (\langle\bar{\psi}\psi\rangle_0 - \langle\bar{\psi}\psi\rangle_T)\frac{m_{ud}}{f_\pi^4}$$



Similar rescalings in the imaginary μ_B direction:
W-B: PRL 126 (2021) 23, 232001; W-B: PRL 125 (2020) 5, 052001;
Also works at real $\mu_B \to$ no sign of a strengthening crossover

Chemical potential scan - 2stout improved $N_\tau = 6$



$T = 140$MeV and $0 \leq \mu_B \leq 380$MeV. The direct method penetrates the region where errors from analytic continuation blow up!

Summary

- Methods to study finite density QCD are typically not bottlenecked by the sign problem itself but other effects
- Observables that are sensitive to criticality are unknown for say $\mu_B/T \geq 1.5$
- We advocate a "new" reweighting method that is free from the overlap problem in the weights and is therefore only bottlenecked by the sign problem itself
- The sign problem is managable for the RHIC BES range
- Penetrates the region where extrapolation methods are not that predictive
- First physics results
- Active research: cutting the costs with algorithmic tricks
  2D scan of the $T - \mu_B$ plane